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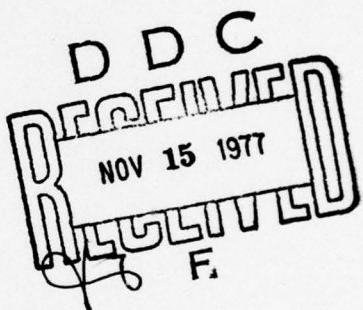
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PERTURBATION OF ELECTRONIC STRUCTURE OF INSULATORS BY INTERFACES AND DEFECT [*]

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Abstract

Extending the theory which developed by Kohn, Onffroy and Rehr for a one-dimensional non-periodic system, we have developed a theory that describes how the electronic density distribution near an insulator-insulator interface approaches the bulk behavior. The exponential decay constant depends on the band structures of the two insulators and the positions of localized surface state energies. In addition, we also study the behavior of the electron density perturbation due to a defect across several successive interfaces.

I. Introduction

In an infinite and perfectly periodic crystal, the eigenfunctions of the one-electron Schrödinger equation are the Bloch waves. The electron density distribution is a periodic function with the same periodicity as the potential. In a crystal with an interface, the periodicity of the potential is lost. The eigenfunctions of this crystal are no longer the Bloch waves. In the vicinity of the interface, the electron density distribution is perturbed by the existence of the interface. However, deep inside each of the crystals, the electron density distribution approaches that of the infinite perfect crystal. In this part, we want to find in what manner the electron density distribution approaches that of the infinite perfect crystal, as we move away from the interface into either of the two crystals. Kohn and Onffroy,[1] Rehr, and Kohn[2] developed a procedure to construct generalized Wannier functions for a system with an impurity or a surface. They found that the generalized Wannier functions approach the Wannier functions of the perfect crystal exponentially with distance from the defect or the surface. We want to extend their idea to study the perturbation of the electron density distribution by an interface in one-dimensional insulators. For an insulator the Fermi level lies at an energy corresponding to a gap for each of the two crystals, i.e. all the energy bands of the perfect crystals are either full or empty. We find that the perturbed electron density distribution approaches that of the perfect crystal in an exponential manner. The decay constant in each crystal is determined by the relative positions of the following quantities: the positions of the band edges of the last filled and first unfilled energy bands of the other crystal; the

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positions of the localized surface state energies; and the position of the branch point energy which are located between the last filled and first unfilled energy bands of this crystal.

We also extend this theory to study more general cases, the way in which the density perturbation due to a defect appears across several successive interfaces. Again, we find that this perturbation decays exponentially and obtain a complete prescription for determining the decay constants for an arbitrary succession of periodic lattices. We believe that our results have some promise for developments of a theory for the following interesting chemical polymer problem: if we replace one atom by a different atom at one point, how does the perturbation behave along the chain of the polymer?

In Section II we will derive the general theory of the electron density perturbation due to the presence of the interface in a one-dimensional insulator of two lattices in contact.

In Section III we will use this theory to discuss the electron density perturbation due to an isolated defect in more complex insulators having n arbitrary different lattices in contact.

Section IV contains a summary of our results.

II. Isolated Defect in a Perfect Insulator and Simple Interface

A. General Theory

Before proceeding to derive the theory, let us briefly review some properties of the perfect periodic lattice.[3] The eigenfunctions of the one-electron Schrödinger equation are the Bloch waves $\psi_n(x,k)$ with energy $E(n,k)$ (eigenvalues). Here k is the wave number and n is the band index. If we treat

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k as a complex variable, $k = g + ih$, then $\Psi_n(x,k)$ and $E(n,k)$ represent the branches of multivalued functions of k. They are analytic everywhere except at a set of branch points away from the real axis. If g is restricted to the fundamental interval $-\frac{\pi}{b} < g \leq \frac{\pi}{b}$, these branch points have the form $k^n = \alpha_n \frac{\pi}{b} \pm ih^n$, where $\alpha_n = 0$ or 1 for n odd or even, respectively. They can be determined from the Kramer's plot (Fig. 1) of $\cos(ka)$ versus real E. The branch points k^n correspond to the $(n+1)$th extremum of this plot. The energy $E_n = E(k^n)$ at these branch points are real.

We now consider an electron in a one-dimensional potential which is taken to be extended over the interval $-d/2 \leq x \leq d/2$, with Hamiltonian (Fig. 2)

$$H = -\frac{d^2}{dx^2} + V(x)$$

$$V(x) = \begin{cases} v_2(x) & -d/2 \leq x < -N \\ v_1(x) & -N \leq x < 0 \\ v_2(x) & 0 \leq x \leq d/2 \end{cases} \tag{2.1}$$

where $v_1(x)$ and $v_2(x)$ are potentials with the periodic and symmetry properties:

$$v_\nu(x+b) = v_\nu(x);$$

$$v_\nu(-x) = v_\nu(x), \text{ where } \nu = 1, 2. \tag{2.2}$$

Here b is the period of the potentials $v_1(x)$ and $v_2(x)$, and where N is the length of the section at which the potential is $v_1(x)$.

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The eigenfunctions $\phi(x)$ are required to satisfy the differential equation:

$$H \phi(x) = E \phi(x) \qquad (2.3)$$

and the conventional periodic boundary conditions:

$$\phi(d/2) = \phi(-d/2) ;$$

$$\qquad (2.4)$$

$$\phi'(d/2) = \phi'(-d/2),$$

where $\phi'(x) \equiv \dfrac{d}{dx} \phi(x)$.

When N equals zero (i.e. the case of the perfect crystal) these eigenfunctions are the Bloch waves

$$\psi_2 (x,k_2), \text{ where } k_2 = \frac{2\pi}{d} \ (- \frac{d}{2b} ,---,0--,(\frac{d}{2b} -1)) . \qquad (2.5)$$

The corresponding eigenvalues are grouped in quasi-continuous energy bands, each containing d/b levels.

When N is not equal to zero, the energy states of the original band split into two groups; one having m localized impurity bands and the other having $(d/b-m)$ minibands (see Fig. 3). When $d \to \infty$, these localized impurity bands approach the bound states and the minibands become scattering states whose energy gaps approach zero[4] (see Fig. 4).

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For real k_2, the electron density contribution of the state $\phi_m(x,k_2)$ in the miniband m is

$$n_m(x,k_2) = \phi_m(x,k_2)\,\phi_m^*(x,k_2) \tag{2.6}$$

where k_2 runs over the fundamental zone $(-\frac{\pi}{d} < k_2 \leq \frac{\pi}{d})$, where m is the index of minibands including the impurity bands and where $\phi_m(x,k_2)$ are ortho-normal Bloch waves, i.e.

$$\int \phi_m^*(x,k_2)\,\phi_{m'}(x,k_2')\,dx = \delta_{mm'}\,\delta(k_2 - k_2'). \tag{2.7}$$

$n_m(x,k_2)$, as defined in Eq. (2.6), is not an analytic function of k_2 because of the complex conjugate appearing in Eq. (2.6). However we know $n_m(x,k_2)$ is independent of the phase of $\phi_m(x,k_2)$. We are then free to choose the phase of $\phi_m(x,k_2)$ such that

$$\phi_m(o,k_2) = \phi_m^*(o,k_2) = \text{real and positive.} \tag{2.8}$$

Then we have the following relations:

$$\phi_m(x,-k_2) = \phi_m^*(x,k_2)\ ;$$

$$\phi_m(-x,k_2) = \phi_m^*(x,k_2). \tag{2.9}$$

If we use the identities of Eq. (2.9) and rewrite Eq. (2.6) in the form

$$n_m(x,k_2) = \phi_m(x,k_2)\,\phi_m(x,k_2)\ , \tag{2.10}$$

then we know that, in this form, n_m (x,k_2) is an analytic function of complex k_2 except at the branch points which connect the miniband m to its neighbors $m \pm 1.$[3]

$$n \ (x,k_2) = \sum_{m=0}^{M} \ n_m \ (x,k_2) \quad ,$$ (2.11)

where m runs over all minibands including the impurity bands and $n \ (x,k_2)$ is analytic at all branch points connecting the minibands m[1].

The total electron density from all the states of this band is

$$n \ (x) = \int_{-\frac{\pi}{d}}^{\frac{\pi}{d}} dk_2 n \ (x,k_2) = \sum_{m=0}^{M} \int_{-\frac{\pi}{d}}^{\frac{\pi}{d}} dk_2 \ n_m \ (x,k_2)$$ (2.12)

as $d \rightarrow \infty$, we have

$$n \ (x) = \int_{-\frac{\pi}{b}}^{\frac{\pi}{b}} dk_2 \ n^{sc} \ (x,k_2) + \sum_{j} n^{B} \ (x,k_2^{\ j})$$ (2.13)

where $n^{sc} \ (x,k_2^{\ j})$ the electron density of the scattering states, is

$$n^{sc} \ (x,k_2) = \psi_{k_2}^{(+)} \ (x) \ \psi_{-k_2}^{(-)} \ (x) \quad ,$$ (2.14)

where $\psi_{\pm k}^{(\pm)} \ (x)$ are the scattering states, $(+)$ and $(-)$ denoting states with outgoing and incoming scattered states, respectively.

$n^{B} \ (x,k_2^{\ j})$, the electron density of the bound states, is

$$n^B (x, k_2{}^j) = \phi^B (x, k_2{}^j) \left[\phi^B (x, k_2{}^j) \right]^* , \qquad (2.15)$$

where $\phi^B (x, k_2{}^j)$ are the normalized bound state wave functions with wave vector $k_2{}^j$ whose amplitudes are determined by the following asymptotic condition:

$$\phi^B (x, k_2{}^j) = \psi_2 (x, k_2{}^j) , \quad x > 0, \qquad (2.16)$$

where $k_2{}^j$ is determined by the relation:

$$E^{(2)} (k_2{}^j) = \varepsilon_j^B \qquad (2.17)$$

and where ε_j^B is the bound state energy which is in the energy gap of a perfect lattice with potential $v_2 (x)$. Here $\sum_j$ extends over all the occupied bound states.

The scattering process due to the existence of the potential $v_1 (x)$ can be described by a transfer matrix $M^{(2)}$ which relates the amplitude and phase of the scattered waves to those of the incident waves. Here the superscript (2) denotes k_2 as an independent variable. We use two different ways to derive the transfer matrix: (1) Saxon's multi-scattering method;[4] (2) Heine's Bloch wave matching method.[5]

(1) Saxon's multi-scattering method:

We can regard the presence of the potential $v_1 (x)$ as a succession of scattering centers which are located from $x = -N$ to $x = 0$ (see Fig. 2). When $N = 1$, the solution can be viewed as an unperturbed Bloch wave interacting with an isolated localized impurity. This scattering process can be described by a scattering matrix $R^{(2)}$ which relates the amplitude and phase of the scattered waves to those of the incident waves. For a finite N , the passage

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of an electron through the N scattering centers can be thought of as a multiple scattering of Bloch electron waves by those scattering centers. The transfer matrix is then

$$M^{(2)} = R^{(2)} S_{-1}^{(2)} (S_{-2}^{(2)})^{-1} R^{(2)} - - - R^{(2)} S_{-(N-1)}^{(2)} (S_{-N}^{(2)})^{-1} R^{(2)} S_{-N}^{(2)}$$

$$= R^{(2)} (G^{(2)})^N S_{-N}^{(2)} \tag{2.18}$$

where $S_a^{(2)}$ is the translation matrix for translation to the right through a lattice constant: (From now on, we assume that the lattice constant b equals one.)

$$S_a^{(2)} = \begin{pmatrix} e^{ik_2 a} & 0 \\ 0 & e^{-ik_2 a} \end{pmatrix} \quad , \tag{2.19}$$

where $R^{(2)}$ has the following properties:

$$R_{11}^{(2)} R_{22}^{(2)} - R_{12}^{(2)} R_{21}^{(2)} = 1 \quad ,$$

$$R_{12}^{(2)} (k_2) = -R_{21}^{(2)} (k_2) \quad ,$$

$$R_{12}^{(2)} (k_2) = R_{21}^{(2)} (-k_2) \quad ,$$

$$R_{11}^{(2)} (k_2) = R_{22}^{(2)} (-k_2) \quad , \tag{2.20}$$

and where

$$G^{(2)} \equiv S_1^{(2)} R^{(2)} \tag{2.21}$$

From Appendix A, we have

$$M^{(2)} = \frac{1}{\alpha}\begin{pmatrix} \{ R_{11}^{(2)} \tfrac{1}{2}\left[(\beta+\alpha)\lambda_1^N - (\beta-\alpha)\lambda_2^N\right] + R_{12}^{(2)} R_{21}^{(2)} e^{-ik_2}(\lambda_1^N - \lambda_2^N)\} e^{-ik_2 N} \\[2mm] \{ R_{21}^{(2)} \tfrac{1}{2}\left[(\beta+\alpha)\lambda_1^N - (\beta-\alpha)\lambda_2^N\right] + R_{22}^{(2)} R_{21}^{(2)} e^{-ik_2}(\lambda_1^N - \lambda_2^N)\} e^{-ik_2 N} \end{pmatrix}$$

$$\{ R_{11}^{(2)} R_{12}^{(2)} e^{ik_2}(\lambda_1^N - \lambda_2^N) + R_{12}^{(2)} \tfrac{1}{2}\left[(\beta+\alpha)\lambda_2^N - (\beta-\alpha)\lambda_1^N\right]\} e^{ik_2 N}$$

(2.22)

$$\{ R_{21}^{(2)} R_{12}^{(2)} e^{ik_2}(\lambda_1^N - \lambda_2^N) + R_{22}^{(2)} \tfrac{1}{2}\left[(\beta+\alpha)\lambda_2^N - (\beta-\alpha)\lambda_1^N\right]\} e^{ik_2 N}$$

where

$$\alpha = \sqrt{\left(R_{11}^{(2)} e^{ik_2} + R_{22}^{(2)} e^{-ik_2}\right)^2 - 4}$$

$$\beta = R_{11}^{(2)} e^{ik_2} - R_{22}^{(2)} e^{-ik_2}$$

$$\lambda_1 = \tfrac{1}{2}\left[\left(R_{11}^{(2)} e^{ik_2} + R_{22}^{(2)} e^{-ik_2}\right) + \alpha\right]$$

$$\lambda_2 = \tfrac{1}{2}\left[\left(R_{11}^{(2)} e^{ik_2} + R_{22}^{(2)} e^{-ik_2}\right) - \alpha\right]$$

(2) Heine's Bloch wave matching method:

We consider a system with three regions (Fig. 2). In regions I and III, the potential is $v_2(x)$ while in region II it is $v_1(x)$. Let $\psi_I(x)$, $\psi_{II}(x)$ and $\psi_{III}(x)$ denote the wave functions in the regions I, II, and III, respectively. Since the potential in regions I and III is $v_2(x)$, $\psi_I(x)$ and $\psi_{II}(x)$ must be linear combinations of the Bloch waves $\psi_2(x, k_2)$. By the same reasoning, $\psi_{II}(x)$ is a linear combination of the Bloch waves $\psi_1(x, k_1)$

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$$\psi_I(x) = a_1 \psi_2(x,k_2) + b_1 \psi_2(x,-k_2)$$

$$\psi_{II}(x) = a_2 \psi_1(x,k_1) + b_2 \psi_2(x,-k_1)$$

$$\psi_{III}(x) = a_3 \psi_2(x,k_2) + b_3 \psi_2(x,-k_2) \tag{2.24}$$

Using the continuity conditions at the interfaces, we obtain

$$M^{(2)} = \frac{1}{W(\psi_1(0,k_1),\psi_1(0,-k_1))\, W(\psi_2(0,k_2),\psi_2(0,-k_2))}$$

$$\times \begin{pmatrix} Q_{22}^{(2)}, & -Q_{12}^{(2)} \\ -Q_{21}^{(2)}, & Q_{11}^{(2)} \end{pmatrix} \begin{pmatrix} e^{i(k_1-k_2)N}Q_{11}^{(2)}, & e^{i(k_1+k_2)N}Q_{12}^{(2)} \\ e^{-i(k_1+k_2)N}Q_{21}^{(2)}, & e^{-i(k_1-k_2)N}Q_{22}^{(2)} \end{pmatrix} \tag{2.25}$$

and

$$E^{(2)}(k_2) = E^{(1)}(k_1) \tag{2.26}$$

where $w(f,g)$ is the Wronskian of the functions f and g :

$$w(f,g) \equiv fg' - f'g \tag{2.27}$$

and where

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$$Q_{11}^{(2)} = w \; (\psi_2(0,k_2), \; \psi_1(0,-k_1) \;)$$

$$Q_{12}^{(2)} = w \; (\psi_2(o,-k_2), \; \psi_1(0,-k_1) \;)$$

$$(2.28)$$

$$Q_{21}^{(2)} = w \; (\psi_1(0,k_1), \psi_2(0,k_2) \;)$$

$$Q_{22}^{(2)} = w \; (\psi_1(0,k_1), \psi_2(0,-k_2) \;)$$

For a finite N , the ratio of the transfer matrix elements $M_{12}^{(2)}/M_{22}^{(2)}$ is an analytic function of k_2, except at branch points which are the same as those of $E^{(2)}$ (k_2) and for the possible pole singularities at the zeroes of $M_{22}^{(2)}$. As N goes to infinity, though the $M_{12}^{(2)}/M_{22}^{(2)}$ retains the just mentioned branch point structure, two additional analytic features arise: (1) two new sets of branch points occur at values of k_2 corresponding to the band edges of a perfect lattice with potential v_1 (x) and (2) an infinite sequence of poles arise from the infinitely many zeroes of $M_{22}^{(2)}$.

The perturbation of electron density at x_2 $(x_2 > 0)$ due to the existence of the potential v_1 (x) is (Appendix B)

$$\delta n(x_2) = \int_{-\frac{\pi}{b}}^{\frac{\pi}{b}} dk_2 \; \frac{M_{12}^{(2)}}{M_{22}^{(2)}} \; \psi_2(x_2,k_2) \; \psi_2(x_2,k_2) + \sum_{j} n^B \; (x_2,k_2^{\;j}) \qquad (2.29)$$

We would like to discuss Eq. (2.29) in the following two simple cases: an isolated defect in a one-dimensional perfect insulator, and an interface.

B. Isolated Defect

When $N = 1$, the system can be thought of as an isolated defect at the origin in a perfect lattice with the potential $v_2(x)$. The strength of the defect potential is $v_1(x)$ (see Fig. 5).

Since $M_{12}^{(2)}/M_{22}^{(2)}$ is regular in the upper half of the k_2 plane in the region between the real axis and the branch points k_2^0, except for the possible pole singularities at zeroes of $M_{22}^{(2)}$ corresponding to the existence of the bound states, we can free to shift the path of integration of Eq. (2.29), from the real axis of k_2 to the contour C as indicated in Fig. 6. This results because of the periodicity of the integrand in Eq. (2.29) (the vertical portions cancel each other).[2] Thus

$$\delta n(x_2) = \int_C dk_2 \; \frac{M_{12}^{(2)}}{M_{22}^{(2)}} \; \psi_2(x_2,k_2)\psi_2(x_2,k_2) + \sum_j n^B(x_2,k_2^j)$$

$$-2\pi i \sum_{j'} \; \text{res} \left[\frac{M_{12}^{(2)}}{M_{22}^{(2)}} \; \psi_2(x_2,k_2^{j'})\psi_2(x_2,k_2^{j'}) \right] \tag{2.30}$$

where j runs over all the occupied bound states and where j' runs over all the poles which are located between the real axis and the contour C.

From Eq. (2.30), $\delta n(x_2)$ will depend upon the strength of $v_1(x)$ and $v_2(x)$, the positions of the zeroes of $M_{22}^{(2)}$ and the positions of the branch points, $E_o^{(2)}$, which are located between the last filled and the first unfilled energy bands of a lattice with the potential $v_2(x)$. We can classify all situations into three cases:

Case 1: $E_o^{(2)}$ lies between the energies of the first unoccupied state and the last occupied state: the residues due to the zeroes of $M_{22}^{(2)}$ precisely cancel the bound state contributions.[2] We obtain

$$\delta n(x_2) = \int_C dk_2 \, \frac{M_{12}^{(2)}}{M_{22}^{(2)}} \, \psi_2(x_2, k_2) \, \psi_2(x_2, k_2) \qquad (2.31)$$

This leads to the asymptotic behavior:

$$|\delta n(x_2)| < (\text{const.}) \, e^{-2h_2^o \, x_2} \quad \text{as } x_2 \to \infty , \qquad (2.32)$$

where h_2^o is the distance from the real axis to the branch points k_2^o in the k_2 plane.

Case 2: $E_o^{(2)}$ lies below the energy of the last occupied state: the residues from the zeroes of $M_{22}^{(2)}$ just cancel these contributions of the bound states the energies of which are lower than $E_o^{(2)}$. $\delta n(x_2)$ becomes

$$\delta n(x_2) = \int_C dk_2 \, \frac{M_{12}^{(2)}}{M_{22}^{(2)}} \, \psi_2(x_2, k_2) \, \psi_2(x_2, k_2) + \sum_j n^B(x_2, k_2^j) \qquad (2.33)$$

$$E^{(2)}(k_2^j) > E_o^{(2)}$$

This leads to the asymptotic behavior:

$$|\delta n(x_2)| < (\text{const.}) \, e^{-2h_2^H \, x_2} \quad \text{as } x_2 \to \infty \qquad (2.34)$$

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where h_2^H is the distance from the real axis to the wave vectors corresponding to the highest occupied state in the k_2 plane.

Case 3: $E_o^{(2)}$ lies above the energy of the first unoccupied state: the bound state contributions of Eq. (2.30) then cancel the residues of the zeroes of $M_{22}^{(2)}$ which are corresponding to the occupied bound states. $\delta n\ (x_2)$ becomes

$$\delta n\ (x_2) = \int_C dk_2\ \frac{M_{12}^{(2)}}{M_{22}^{(2)}}\ \psi_2\ (x_2,k_2)\ \psi_2(x_2,k_2)$$

$$-2\pi i \sum_{j'} \text{res} \left[\frac{M_{12}^{(2)}}{M_{22}^{(2)}}\ \psi_2\ (x_2,k_2^{j'})\ \psi_2\ (x_2,k_2^{j'}) \right] \qquad (2.35)$$

where j' runs over all poles of $M_{22}^{(2)}$ corresponding to the unoccupied bound states the energies of which are lower than $E_o^{(2)}$. This leads to the asymptotic behavior:

$$|\delta n(x_2)| \ <\ (\text{const.})\ e^{-2h_2^L x_2} \qquad \text{as } x_2 \to \infty \qquad (2.36)$$

where h_2^L is the distance from the real axis to the wavevectors corresponding to the first unoccupied state.

C. Simple Interface:

As the length of the potential $v_1(x)$ goes to infinity $(N \to \infty)$, the system shown in Fig. 2 looks like two one-dimensional periodic lattices joined at the origin (Fig. 6). In this case, $M_{12}^{(2)}/M_{22}^{(2)}$ is an analytic function of k_2 except at branch points which are the same as those of $E^{(2)}(k_2)$, at wavevectors corresponding to the band edges of a perfect lattice with the potential $v_1(x)$ and at the infinitely many pole singularities which occur at the zeroes of $M_{22}^{(2)}(k_2)$ (which corresponds to the existence of the bound states).

Because of this analyticity and the periodic properties of the integrand of Eq. (2.30), we can shift the path of integration from the real axis to the contour C as indicated in Fig. 8. The change of the electron charge density at x_2 is (Appendix B)

$$\delta n(x_2) = \int_C dk_2 \frac{M_{12}^{(2)}}{M_{22}^{(2)}} \psi_2(x_2, k_2) \psi_2(x_2, k_2) + \sum_j n^B(x_2, k_2^j)$$

$$-2\pi i \sum_{j'} \text{res} \left[\frac{M_{12}^{(2)}}{M_{22}^{(2)}} \psi_2(x_2, k_2^{j'}) \psi_2(x_2, k_2^{j'}) \right] \qquad (2.37)$$

The second term on the right hand side of Eq. (2.37) is the contribution from all the occupied bound states which are located in the gap between the first unfilled and last filled band of a perfect lattice with potential $v_2(x)$. The third term is the contribution from the poles from the zeroes of $M_{22}^{(2)}$ which are located between the real k_2 axis and the contour C.

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Again, we can discuss Eq. (2.37) in three cases as we did for the isolated defect.

Case 1: $E_o^{(2)}$ lies between the energies of the first unoccupied state and the last occupied state: the second and the third terms on the right hand side of Eq. (2.37) then cancel each other identically. $\delta n (x_2)$ becomes

$$\delta n (x_2) = \int_C dk_2 \frac{M_{12}^{(2)}}{M_{22}^{(2)}} \psi_2 (x_2, k_2) \psi_2 (x_2, k_2) \tag{2.38}$$

We then have the asymptotic behavior:

$$|\delta n (x_2)| < (\text{const.}) e^{-2h_2^o x_2} \quad \text{as } x_2 \to \infty \quad . \tag{2.39}$$

Case 2: $E_o^{(2)}$ lies below the energy of the last occupied state: the third term on the right hand side of Eq. (2.37) then just cancels the contribution of the bound states the energies of which are lower than $E_o^{(2)}$. $\delta n (x_2)$ becomes

$$\delta n (x_2) = \int dk_2 \frac{M_{12}^{(2)}}{M_{22}^{(2)}} \psi_2 (x_2, k_2) \psi_2 (x_2, k_2) + \sum_j n^B (x_2, k_2^j) \tag{2.40}$$

$$E^{(2)} (k_2^j) > E_o^{(2)} .$$

We then have the asymptotic behavior:

$$|\delta n (x_2)| < (\text{const.}) e^{-2h_2^H x_2} , \text{ as } x_2 \to \infty \quad . \tag{2.41}$$

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Case 3: $E_o^{(2)}$ lies above the energy of the first unoccupied state: the second term on the right hand side of Eq. (2.37) then cancels all the residues from the poles corresponding to the occupied bound states. $\delta n (x_2)$ becomes

$$\delta n (x_2) = \int_C dk_2 \frac{M_{12}^{(2)}}{M_{22}^{(2)}} \psi_2 (x_2, k_2) \psi_2 (x_2, k_2) -2\pi i \sum_{j'} \text{res} \left[\frac{M_{12}^{(2)}}{M_{22}^{(2)}} \psi_2 (x_2, k_2^{j'}) \psi_2 (x_2, k_2^{j'}) \right] . \tag{2.42}$$

where j' runs over all the poles corresponding to the unoccupied bound states the energies of which are lower than $E_o^{(2)}$. We then have the asymptotic behavior:

$$|\delta n (x_2)| < (\text{const.}) \, e^{-2h_2^L \, x_2} \quad \text{as } x_2 \to \infty . \tag{2.43}$$

We, therefore, have concluded that the electron density distribution moving away from the interface approaches exponentially the bulk values. The decay constant depends upon the relative position of the band structure of the perfect lattices.

III. <u>More General Systems</u>

In this Section, we extend the theory developed in Section II to study the following question: if a point perturbing potential is introduced into a system which contains a succession of n arbitrary different insulators as shown in Fig. 9, how does the electron density perturbation produced by this disturbance appear across successive interfaces?

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First, let us consider the simplest case: a system with just one interface. We take the perturbing potential (defect) at point P a distance x_1 to the left of the interface as indicated in Fig. 10.

To obtain the transfer matrix of the system, we will follow the Saxon's method as we did before. In this method, we only replace the scattering matrix $R^{(2)}$ at $x = -x_1$ (see Eq. (2.23)) by the defect scattering matrix $T^{(2)}$. Then the transfer matrix of the system with the defect is

$$M_I^{(2)} = R^{(2)} \; (S_1^{(2)} \; R^{(2)})^{x_1} \; (S_1^{(2)} \; T^{(2)}) \; (S_1^{(2)} \; R^{(2)})^{N-x_1-1} \; S_{-N}^{(2)} \; . \quad (3.1)$$

and that without the defect is

$$M^{(2)} = R^{(2)} \; (S_1^{(2)} \; R^{(2)})^{x_1} \; (S_1^{(2)} R^{(2)}) \; (S_1^{(2)} \; R^{(2)})^{N-x_1-1} \; S_{-N}^{(2)} \; . \quad (3.2)$$

The analytic properties of the $M_{I,12}^{(2)}/M_{I,22}^{(2)}$ are similar to those of the $M_{12}^{(2)}/M_{22}^{(2)}$: both are analytic functions except at branch points and poles as discussed above in the case of the simple interface. However, though the branch points occur at the same k_2 values for both functions, the poles occur at different k_2 values (the zeroes of $M_{I,22}^{(2)}$ in general differ from those of $M_{22}^{(2)}$) .

Using the same procedure as we followed for the case of the simple interface, we have the following form for the change of the electron density distribution at a distance x_2 to the right of the interface due to a defect at a distance

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x_1 to the left of the interface

$$\delta n \ (x_1, \ x_2) \equiv n_I \ (x_1, x_2) - n \ (x_1, \ x_2)$$

$$= \int_C dk_2 \ (\frac{M_{I,12}^{(2)}}{M_{I,22}^{(2)}} - \frac{M_{12}^{(2)}}{M_{22}^{(2)}}) \ \psi_2 \ (x_2, k_2) \psi_2 \ (x_2, k_2)$$

$$+ \sum_j n_I^B \ (x_2, k_2^{\ j}) - \sum_j n^B \ (x_2, k_2^{\ j})$$

$$- 2\pi i \ \left\{ \sum_{j'} \ \text{res} \ \left[\frac{M_{I,12}^{(2)}}{M_{I,22}^{(2)}} \ \psi_2 \ (x_2, k_2^{\ j'}) \psi_2 (x_2, k_2^{\ j'}) \right] \right.$$

$$\left. - \sum_{j'} \ \text{res} \ \left[\frac{M_{12}^{(2)}}{M_{22}^{(2)}} \ \psi_2 \ (x_2, k_2^{\ j'}) \psi_2 (x_2, k_2^{\ j'}) \right] \right\}$$

$$\tag{3.3}$$

where the subscript I denotes the system with a defect; the notation otherwise being the same as in Section II.

By the same reasoning which we used to discuss Eq. (2.37), we find that $n \ (x_1, x_2)$ has the following asymptotic behavior:

$$|\delta n \ (x_1, x_2)| < (\text{const.})_{x_1} \ e^{-2\alpha_2 x_2} \ \text{as} \ x_2 \to \infty \tag{3.4}$$

where the subscript x_1 indicates x_1 kept constant in this equation. α_2 is the decay constant in the insulator 2; it has different values for the following three cases:

Case 1: When the energy of the first unoccupied state is higher than $E_o^{(2)}$ and the energy of the last occupied state is lower than $E_o^{(2)}$,

$$\alpha_2 = h_2^{\;o} \quad . \tag{3.5}$$

Case 2: When the energy of the last occupied state is higher than $E_o^{(2)}$,

$$\alpha_2 = h_2^{\;H} \quad . \tag{3.6}$$

Case 3: When the energy of the first unoccupied state is lower than $E_o^{(2)}$,

$$\alpha_2 = h_2^{\;L} \quad . \tag{3.7}$$

If in case (2) the bound state from the defect is the last occupied state or if in case (3) it is the first unoccupied state, then α_2 depends upon the strength of the defect potential. Otherwise α_2 depends upon the potentials of the two lattices only.

We now want to discuss the modification of $\delta n \, (x_1, x_2)$ as the defect is moved away from the interface while x_2 is fixed. To obtain the functional dependence of $\delta n \, (x_1, x_2)$ upon x_1, we have to change the fundamental interval in Fig. 2 as follows: it is taken to be a perfect lattice with potential $v_1 \, (x)$ with extended impurities from $x = 0$ to $x = N$ of the potential $v_2 \, (x)$ as indicated in Fig. 11. The potential in this fundamental interval is given by

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$$V(x) \begin{cases} v_1(x) & -d/2 \le x < 0 \\ \\ v_2(x) & 0 \le x < N \\ \\ v_1(x) & N \le x < d/2 \end{cases} \tag{3.8}$$

Using the same procedure as before, we obtain the transfer matrix of this system by Saxon's method;

$$M_I^{(1)} = S_{N+1}^{(1),-1} (S_1^{(1)} R^{(1)})^{N-x_2} S_{x_2+1}^{(1)} S_{x_2+1}^{(1),-1} (S_1^{(1)} R^{(1)})^{x_2+1}$$

$$S_{-x_1}^{(1),-1} T^{(1)} S_{-x_1}^{(1)} \tag{3.9}$$

and

$$M^{(1)} = S_{N+1}^{(1),-1} (S_1^{(1)} R^{(1)})^{N-x_2} S_{x_2+1}^{(1)} S_{x_2+1}^{(1),-1} (S_1^{(1)} R^{(1)})^{x_2+1} \tag{3.10}$$

All the notation is the same as before, except for the superscript (1) which denotes k_1 as an independent variable.

From the Appendix D, we obtain the following asymptotic behavior of $\delta n (x_1, x_2)$ with fixed x_2

$$|\delta n (x_1, x_2)| < (\text{const.})_{x_2} e^{-2\alpha_1 x_1} \text{ as } x_1 \to \infty \tag{3.11}$$

where α_1 is the decay constant in the insulator 1. It is given by

1) $\alpha_1 = h_1^O$,

if the energy of the first unoccupied state is higher than $E_o^{(1)}$ and the energy of the last occupied state is lower than $E_o^{(1)}$.

2) $\alpha_1 = h_1^H$,

if the energy of the last occupied state is higher than $E_o^{(1)}$.

3) $\alpha_1 = h_1^L$,

if the energy of the first unoccupied state is lower than $E_o^{(1)}$.

where $E_o^{(1)}$, the branch points of the energy surface $E^{(1)}(k_1)$, is located between the first unfilled and last filled band of a perfect lattice with potential $v_1(x)$. h_1^O , h_1^H and h_1^L are the distances from the real axis to the wavevectors corresponding to the branch points, the last occupied state, and the first unoccupied state, respectively.

From Eqs: (3.4) and (3.11), we have the following asymptotic behavior of $\delta n(x_1, x_2)$:

$$|\delta n(x_1, x_2)| < (\text{const.}) \ e^{-2\alpha_1 x_1} \ e^{-2\alpha_2 x_2} \quad \text{as } x_1 \to \infty$$

$$x_2 \to \infty \qquad (3.12)$$

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We now want to discuss the effect of a defect in a more general system, namely, a system with n interfaces. This system has a succession of $n+1$ arbitrary different sublattices as shown in Fig. 9. The potential in the νth sublattice is denoted by $v_\nu(x)$. All the sublattices except for those at the ends are of finite length, denoted by x_ν; the end lattices are infinite. We put an isolated defect in the first sublattice at a distance x_1 to the left of the interface which divides the first and second sublattices. We want to determine the change of the electron density distribution, $\delta n(x_1, x_2 \ldots, x_{n+1})$, in the last $(\nu=n+1)$ sublattice.

If the length of each sublattice is fixed, we have from the above discussion the following asymptotic behavior of $\delta n(x_1, x_2 \ldots, x_{n+1})$ with respect to x_1 and x_{n+1}:

$$|\delta n(x_1, x_2, \ldots, x_{n+1})| < (\text{const.}) x_2, \ldots, x_n \, e^{-2\alpha_1 x_1} \, e^{-2\alpha_{n+1} x_{n+1}}$$

$$\text{as } x_1 \to \infty$$

$$x_{n+1} \to \infty \qquad (3.13)$$

We now want to find the functional dependence of $\delta n(x_1, x_2, \ldots, x_{n+1})$ upon x_ν for $\nu = 2, 3 \ldots, n$. First, we fix all x_ν except a particular one μ. In this case we can think of the lattice μ as a host lattice while the other lattices are thought of as extended impurities. We choose the fundamental interval shown in Fig. 12 and follow the same procedures as we followed in Sec. II. We have (see Appendix D)

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$$\left| \delta n \left(x_1, x_2, \ldots, x_{n+1} \right) \right| < \text{(const.)} \ x_1, x_2, \ldots, x_{\mu-1}, x_{\mu+1}, \ldots, x_{n+1} \ e^{-2\alpha_\mu x_\mu} \quad \text{as} \ x_\mu \to \infty$$

(3.14)

where α_μ, the decay constant, has the similar definition as before.

Then we have the following results for the change of the electron density distribution due to a defect:

$$\left| \delta n \left(x_1, x_2, \ldots, x_{n+1} \right) \right| < \text{(const.)} \prod_{\nu=1}^{n+1} e^{-2\alpha_\nu x_\nu} \quad \text{as} \ x_\nu \to \infty$$

(3.15)

where α_ν is the decay constant in the sublattice ν. Its value is given by

1) $\alpha_\nu = h_\nu^{\ o}$,

if the energy of the last occupied state is lower than $E_o^{(\nu)}$ and the energy of the first unoccupied state is higher than $E_o^{(\nu)}$.

2) $\alpha_\nu = h_\nu^{\ H}$,

if the energy of the last occupied state is higher than $E_o^{(\nu)}$.

3) $\alpha_\nu = h_\nu^{\ L}$,

if the energy of the first unoccupied state is lower than $E_o^{(\nu)}$.

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where $E_0{}^{(\nu)}$, the branch points of the energy surface $E^{(\nu)}(k_\nu)$, is located between the first unfilled and last filled energy band of a perfect lattice with potential $v_\nu(x)$. $h_\nu{}^O$, $h_\nu{}^H$, and $h_\nu{}^L$ are the distances from the real axis to the wavevectors corresponding to the branch points, the last occupied state and the first unoccupied state, respectively.

IV. Summary

The perturbation of the electron density distribution due to an isolated defect appearing across $n+1$ successive arbitrary different lattices decays exponentially. The decay constant in a particular sublattice μ depends on the position of the branch points $E_0{}^{(\mu)}$ (which are located between the last filled and first unfilled energy bands of a perfect lattice with potential $v_\mu(x)$.) relative to the energies of the highest occupied state and the last unoccupied state of this system.

There are three cases:

Case 1: If the energy of the last occupied state is lower than $E_0{}^{(\mu)}$ and the energy of the first unoccupied state is higher than $E_0{}^{(\mu)}$, the decay constant equals the distance from the real axis to the wavevectors corresponding to the branch points $E_0{}^{(\mu)}$ in the k_μ plane.

Case 2: If the energy of the last occupied state is higher than $E_0{}^{(\mu)}$, the decay constant equals the distance from the real axis to the wavevectors corresponding to the last occupied state in the k_μ plane.

Case 3: If the energy of the first unoccupied state is lower than $E_0{}^{(\mu)}$, the decay constant equals the distance from the real axis to the wavevectors corresponding to the first unoccupied state in the k_μ plane.

APPENDIX A

In this appendix, we want to discuss the analytic properties of the transfer matrix M (see Eq. (2.18)) for a system with an interface. (For simplicity of notation, the superscript (2) will be suppressed in this appendix.)

To calculate G^N, we have to find a transformation P such that G is in diagonal form:

$$P = \begin{pmatrix} \tfrac{1}{2}(\beta+\alpha), & \tfrac{1}{2}(\beta-\alpha) \\ R_{21}e^{-ik_2}, & R_{21}e^{-ik_2} \end{pmatrix} \tag{A.1}$$

where α and β are defined in Eq. (2.23). G can be written as

$$G = P \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} P^{-1} \tag{A.2}$$

where λ_1 and λ_2 are defined in Eq. (2.23) and where P^{-1} is the inverse matrix of P given by

$$P^{-1} = \frac{1}{|P|} \begin{pmatrix} R_{21}e^{-ik_2} & -\tfrac{1}{2}(\beta-\alpha) \\ -R_{21}e^{-ik_2} & \tfrac{1}{2}(\beta-\alpha) \end{pmatrix} . \tag{A.3}$$

Here $|P|$ is the determinant of P given by

$$|P| = R_{21}e^{-ik_2}\,\alpha. \tag{A.4}$$

From Eq. (A.1) and Eq. (A.2), M can be written as Eq. (2.22).

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We now want to discuss the analytic properties of M_{12}/M_{22} for a system with an interface ($N \to \infty$). From Eq. (2.22), M_{12}/M_{22} is given by

$$\frac{M_{12}}{M_{22}} = \frac{R_{11}R_{12}e^{ik_2}(\lambda_1^N - \lambda_2^N) + R_{12}\frac{1}{2}\left[(\beta+\alpha)\lambda_2^N - (\beta-\alpha)\lambda_1^N\right]}{R_{21}R_{12}e^{ik_2}(\lambda_1^N - \lambda_2^N) + R_{22}\frac{1}{2}\left[(\beta+\alpha)\lambda_2^N - (\beta-\alpha)\lambda_1^N\right]}. \qquad (A.5)$$

Before proceeding with the discussion, let us give the physical meaning of λ_1 and λ_2. By comparing the Saxon's method with the Heine's method we have the following relations between k_1 and k_2:

$$R_{11}e^{ik_2} + R_{22}e^{-ik_2} = e^{ik_1} + e^{-ik_1} ,$$

$$\sqrt{(R_{11}e^{ik_2} + R_{22}e^{-ik_2})^2 - 4} = e^{ik_1} - e^{-ik_1} , \qquad (A.6)$$

where k_1 satisfies the following relation:

$$E^{(2)}(k_2) = E^{(1)}(k_1) . \qquad (A.7)$$

Here $E^{(1)}(k_1)$ and $E^{(2)}(k_2)$ are the energy surfaces of the perfect lattices with the potential $v_1(x)$ and $v_2(x)$, respectively.

Following those relations, λ_1 and λ_2 can be written as:

$$\lambda_1 = e^{ik_1}$$

$$\lambda_2 = e^{-ik_1} \qquad (A.8)$$

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Let us now return to the discussion. M_{12}/M_{22} is an analytic function of k_2, except at its branch points which are the same as those of $E^{(2)}(k_2)$ and which occur for those values of k_2 which correspond to k_1 being $n\pi; n = 0, \pm 1, \pm 2, \cdots (\alpha = 0)$, and has infinitely many poles which occur for those values of k_2 which correspond to the real k_1, i.e. those poles occur at the points corresponding to the points in the allowed bands of $E^{(1)}(k_1)$ and the branch points occur at the points corresponding to the band edges of $E^{(1)}(k_1)$.

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We consider here a one-dimensional lattice to which extended impurities have been added (see Fig. 2). The eigenstates of the system are the scattering states $\psi_{\pm} k_2{}^{(\pm)} (x)$ and the bound states $\phi^B (x, k_2{}^j)$. Here (+) and (-) denote states with outgoing and incoming scattered waves, respectively. Outside the impurity region, the scattering states are appropriate linear combination of Bloch waves:[1]

$$\psi_{k_2}{}^{(+)} (x) = \frac{1}{(M_{22}{}^{(2)})^{\frac{1}{2}}} \begin{cases} \psi_2(x, k_2) & x > 0 \\ M_{22}{}^{(2)} \psi_2(x, k_2) + M_{12}{}^{(2)} \psi_2 (x, -k_2) & x < -N \end{cases}$$

$$\psi_{-k_2}{}^{(+)} (x) = \frac{1}{(M_{22}{}^{(2)})^{\frac{1}{2}}} \begin{cases} M_{22}{}^{(2)} \psi_2 (x, -k_2) + M_{12}{}^{(2)} \psi_2(x, k_2) & x > 0 \\ \psi_2(x, -k_2) & x < -N \end{cases}$$

(B.1)

The coefficients $M_{22}{}^{(2)}$ and $M_{12}{}^{(2)}$ are the elements of the transfer matrix.

At point x_2 $(x_2 > 0)$, the change of electron density due to those impurities is

$$\delta n(x_2) \equiv n_I(x_2) - n(x_2)$$

$$= \int_{-\frac{\pi}{b}}^{\frac{\pi}{b}} dk_2 \, \psi_{k_2}{}^{(+)} (x_2) \, \psi_{-k_2}{}^{(-)} (x_2) + \sum_j n^B (x_2, k_2{}^j)$$

$$- \int_{-\frac{\pi}{b}}^{\frac{\pi}{b}} dk_2 \, \psi_2(x_2,k_2) \, \psi_2(x_2,-k_2)$$

$$= \int_{-\frac{\pi}{b}}^{\frac{\pi}{b}} dk_2 \, \frac{M_{12}^{(2)}}{M_{22}^{(2)}} \, \psi_2(x_2,k_2) \, \psi_2(x_2,k_2) + \sum_j n^B (x_2,k_2^{\,j}) \qquad \text{(B.2)}$$

From Appendix A, we know $M_{12}^{(2)}/M_{22}^{(2)}$ is an analytic function of k_2, except at an infinite number of poles which occur at the zeroes of $M_{22}^{(2)}$, at three sets of the branch points which occur at the points $k_2^{\,o}$, $k_2^{\,\alpha}$ and $k_2^{\,\beta}$, corresponding to the branch points of the energy surface $E^{(2)}(k_2)$, and at the upper and lower band edges of a perfect lattice with the potential $v_1(x)$. If we deform the path of integration of the integral in Eq. (B.2) from the real axis to the contour C just below the branch points $k_2^{\,o}$, the integral in Eq. (B.2) can be written as a single integral along the contour C plus the residues at the zeroes of $M_{22}^{(2)}$ which are located between the real axis and the contour C. This results because of the calculation of the vertical portions of the contour (this is due to the periodicity of the integrand in k_2). $\delta n(x_2)$ becomes

$$\delta n(x_2) = \int_C dk_2 \, \frac{M_{12}^{(2)}}{M_{22}^{(2)}} \, \psi_2(x_2,k_2) \, \psi_2(x_2,k_2) + \sum_j n^B (x_2,k_2^{\,j})$$

$$-2\pi i \sum_{j'} \text{res}\left[\frac{M_{12}^{(2)}}{M_{22}^{(2)}} \, \psi_2 (x_2,k_2^{\,j'}) \, \psi_2 (x_2,k_2^{\,j'}) \right] \qquad \text{(B.3)}$$

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Again, from the appendix A , we know the integral in Eq. (B.3) has the following asymptotic behavior:

$$| \int_C dk_2 \frac{M_{12}^{(2)}}{M_{22}^{(2)}} \psi_2 (x_2,k_2) \psi_2(x_2,k_2) | < (const.) \, e^{-2h_2^{o}x_2} \quad \text{as } x_2 \rightarrow \infty \quad (B.4)$$

where h_2^{o} is the distance from the real axis to the branch points k_2^{o}.

The bound state contributions to $\delta n(x_2)$ are denoted by $\Sigma_j \, n^B(x_2,k_2^{j})$, where j runs over all the occupied bound states and $n^B(x_2,k_2^{j})$ is bounded by (const.) $\exp(-2h_2^{j}x_2)$. Here h_2^{j} is the distance from the real axis to the wave vectors k_2^{j} corresponding to the bound state j with energy $\varepsilon_j^{B} = E^{(2)}(k_2^{j})$.

The residues at the zeroes of $M_{22}^{(2)}$ are denoted by the second summation on the right hand side of Eq. (B.3). j' runs over all the zeroes of $M_{22}^{(2)}$ which are located between the real axis and the contour C . The residue at the zero of $M_{22}^{(2)}$ $k_2^{j'}$ is bound by (const.) $\exp(-2h_2^{j'}x_2)$, where $h_2^{j'}$ is the distance from the real axis to the $k_2^{j'}$.

We will discuss Eq. (B.3) in the following three situations:

(1) if the energy of the last occupied state is lower than $E_o^{(2)}$ and the energy of the first unoccupied state is higher than $E_o^{(2)}$, j and j' on the right hand side of Eq. (B.3) run over the same set of k_2 . The bound state contributes to $\delta n(x_2)$ precisely cancel the residues at the zeroes of $M_{22}^{(2)}$.[1] Therefore, $\delta n(x_2)$ has the following asymptotic behavior:

$$|\delta n(x_2)|<(const.)e^{-2h_2^{o}x_2} \quad \text{as } x_2 \rightarrow \infty \quad (B.5)$$

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(2) If the energy of the last occupied state is higher than $E_o^{(2)}$, the residens at the zeroes of $M_{22}^{(2)}$ between the real axis and the contour C will cancel the contributions of the bound states with energy levels below $E_o^{(2)}$. Eq. (B.3) becomes

$$\delta n(x_2) = \int_C dk_2 \frac{M_{12}^{(2)}}{M_{22}^{(2)}} \psi_2(x_2,k_2)\psi_2(x_2,k_2) + \sum_j n^B(x_2,k_2^j)$$

$$E^{(2)}(k_2^j) > E_o^{(2)} \qquad (B.6)$$

In the forbidden region where the energy is higher than $E_o^{(2)}$, we know from the Kramer's plot that the higher the energy of a bound state, the smaller the distance from the real axis to the wavevectors corresponding to this bound state. Then $\delta n(x_2)$ has the following asymptotic behavior:

$$|\delta n(x_2)| < (const.)\, e^{-2h_2^H x_2} \quad \text{as } x_2 \to \infty \qquad (B.7)$$

where h_2^H is the distance from the real axis to the wavevectors corresponding to the highest occupied state.

(3) If the energy of the lowest unoccupied state is lower than $E_o^{(2)}$, the second term on the right hand side of Eq. (B.3) (the contributions from the occupied bound state) will cancel the residues at the poles corresponding to the occupied bound states. $\delta n(x_2)$ becomes

$$\delta n(x_2) = \int_C dk_2 \frac{M_{12}^{(2)}}{M_{22}^{(2)}} \psi_2(x_2,k_2)\psi_2(x_2,k_2)$$

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$$-2\pi i \sum_{j'} \text{res} \left[\frac{M_{12}^{(2)}}{M_{22}^{(2)}} \psi_2 (x_2, k_2^{j'}) \psi_2 (x_2, k_2^{j'}) \right] \qquad (B.8)$$

where j' runs over all the zeroes of $M_{22}^{(2)}$ corresponding to the unoccupied bound states with energy levels below $E_o^{(2)}$.

In the forbidden region where the energy is lower than $E_o^{(2)}$, we know from the Kramer's plot that the higher the energy of a bound state, the larger the distance from the real axis to the wavevectors corresponding to this bound state. Then $\delta n(x_2)$ has the following

$$|\delta n(x_2)| < (\text{const.}) \, e^{-2h_2^L x_2} \quad \text{as } x_2 \to \infty \qquad (B.9)$$

where h_2^L is the distance from the real axis to the wavevectors corresponding to the lowest unoccupied state.

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In this appendix, we want to derive Eq. (3.11). If we define A, A_I and B as follows:

$$A = S_{x_2+1}^{-1} \ (S_1 R)^{x_2+1}$$

$$A_I = S_{x_2+1}^{-1} (S_1 R)^{x_2+1} \ S_{-x_1}^{-1} \ T \ S_{-x_1}$$

$$B = S_{N+1}^{-1} \ (S_1 R)^{-x_2} \ S_{x_2+1} \ ,$$ (C.1)

the M_I and M defined in Eqs. (3.9) and (3.10) can be written as:

$$M_I = B \cdot A_I$$

$$M = B \cdot A$$ (C.2)

Again, for simplicity of notation, we suppress the superscript (1) in this appendix.

The change of the electron density distribution at the point x_2 due to the defect at the point x_1 is

$$\delta n(x_1, x_2) = \int_{-\frac{\pi}{b}}^{\frac{\pi}{b}} dk_1 \left[\psi_{I,k_1}^{(+)}(x_2) \psi_{I,-k_1}^{(-)}(x_2) - \psi_{k_1}^{(+)}(x_2) \psi_{-k_1}^{(-)}(x_2) \right]$$

$$+ \sum_j n_I^B (x_2, k_1^j) - \sum_j n^B(x_2, k_1^j) \ ,$$ (C.3)

where $\psi_{I',\pm k_1}^{(+)}(x)$ are the scattering states of the system with the defect:

$$\psi_{I,k_1}^{(+)}(x_2) = \frac{1}{(M_{I,22})^{\frac{1}{2}}} \left[B_{22}\,\psi_1(x_2,k_1) - B_{21}\,\psi_1(x_2,-k_1) \right]$$

$$\psi_{I,-k_1}^{(-)}(x_2) = \frac{1}{(M_{I,22})^{\frac{1}{2}}} \left[A_{I,12}\,\psi_1(x_2,k_1) + A_{I,22}\,\psi_1(x_2,-k_1) \right] \qquad (C.4)$$

and where $\psi_{\pm k_1}^{(+)}(x)$ are the scattering states of the system without the defect:

$$\psi_{k_1}^{(+)}(x_2) = \frac{1}{(M_{22})^{\frac{1}{2}}} \left[B_{22}\,\psi_1(x_2,k_1) - B_{21}\psi_1(x_2,-k_1) \right]$$

$$\qquad (C.5)$$

$$\psi_{-k_1}^{(-)}(x_2) = \frac{1}{(M_{22})^{\frac{1}{2}}} \left[A_{12}\,\psi_1(x_2,k_1) + A_{22}\psi_1(x_2,-k_1) \right]$$

The integrand of the Eq. (C.3) $I(x_1,x_2,k_1)$ can be written as:

$$I(x_1,x_2,k_1) = \frac{1}{M_{I,22}} \left[B_{22}\psi_1(x_2,k_1) - B_{21}\psi_1(x_2,-k_1) \right]\left[A_{I,12}\psi_1(x_2,k_1) \right.$$

$$\left. - A_{I,22}\psi_1(x_2,-k_1) \right] - \frac{1}{M_{22}} \left[B_{22}\psi_1(x_2,k_1) - B_{21}\psi_1(x_2,-k_1) \right]$$

$$\left[A_{12}\psi_1(x_2,k_1) - A_{22}\psi_1(x_2,-k_1) \right]$$

$$= \frac{1}{M_{22}M_{I,22}} (A_{I,12}A_{22} - A_{12}A_{I,22}) \left[B_{22}\psi_1(x_2,k_1) - B_{21}\psi_1(x_2,-k_1) \right]^2$$

$$= T_{12}\, e^{2ik_1 x_1} \left[G_{22}^{N-x_2}\, e^{-ik_1(x_2+1)}\, \psi_1(x_2,k_1) - G_{21}^{N-x_2} \right.$$

$$\left. e^{ik_2(x_2+1)}\, \psi_1(x_2,-k_1) \right]^2 \Big/$$

$$\{\left[G_{21}^{N-x_2} \, (T_{12}G_{11}^{x_2+1} \, e^{2ik_1x_1} + T_{22}G_{12}^{x_2+1}) + G_{22}^{N-x_2} \, (T_{12}G_{21}^{x_2+1} \, e^{2ik_1x_1}$$

$$+ T_{22}G_{22}^{x_2+1})\right] \left[G_{21}^{N-x_2} \, G_{12}^{x_2+1} + G_{22}^{N-x_2} G_{22}^{x_2+1}\right]\},$$

where $G \equiv S_1 R$.

$I(x_1, x_2, k_1)$ has the same analytic properties as the integrand of Eq. (B.2). We can deform the path of integration of the integral in Eq. (C.3) to a contour C just below the branch points of $E^{(1)}(k_1)$ as we did in Appendix B. We obtain the asymptotic behavior of the following integral along the contour C with fixed x_2:

$$\left| \int_C dk_1 I(x_1, x_2, k_1) \right| < (\text{const.})_{x_2} \, e^{-2h_1^{\,o}x_1} \quad \text{as } x_1 \to \infty \tag{C.7}$$

where $h_1^{\,o}$ is the distance from the real axis to the wavevectors corresponding to the branch points of $E^{(1)}(k_1)$.

Using Eq. (C.7) and following the same reasoning as we did in Appendix B, we can obtain Eq. (3.11).

APPENDIX D

In this appendix, we want to derive Eq. (3.14). For simplicity, we consider here the system with two interfaces as shown in Fig. 9 instead of n interfaces. There are three sublattices 1, 2 and 3 with the potential $v_1(x)$, $v_2(x)$ and $v_3(x)$, respectively. Since we want to obtain the asymptotic behavior of the change of the electron density distribution in the sublattice 3 due to a defect in the sublattice 1 as the length of the sublattice 2 x_2 approaches to infinity, we can think of the sublattice 2 as a host lattice and k_2 as an independent variable while the other sublattices 1 and 3 are thought of as extended impurities. The fundamental interval of this system is shown in Fig. 11. The lengths of the sublattices 1 and 3 are denoted by ℓ_1 and ℓ_3, respectively.

The transfer matrices for this system with and without the defect are given by

$$M_I = B \cdot A_I$$

$$M = B \cdot A \tag{D.1}$$

where

$$B = S_{\ell_3}^{-1} (S_1 K)^{\ell_3 - x_3} S_{x_3}$$

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$$A_I = S_{x_3}^{-1} (S_1 K)^{x_3} S_{-x_2}^{-1} (S_1 R)^{x_1 - 1} (S_1 T)(S_1 R)^{\ell_1 - x_1} S_{-(\ell_1 + x_2)}$$

$$A = S_{x_3}^{-1} (S_1 K)^{x_3} S_{-x_2}^{-1} (S_1 R)^{\ell_1} S_{-(\ell_1 + x_2)} \quad . \tag{D.2}$$

Here R and K are the scattering matrices due to a localized impurity at the origin in a perfect lattice 2 with the impurity strength $v_1(x)$ and $v_3(x)$, respectively and where the point x_3 is in the sublattice 3 and the point x_1 is in the sublattice 1.

The change of the electron density distribution at the point x_3 due to the defect at the point x_1 is given by

$$\delta n(x_1, x_2, x_3) = \int_{-\frac{\pi}{b}}^{\frac{\pi}{b}} dk_2 \frac{1}{M_{I,22} M_{22}} (A_{I,12} A_{22} - A_{12} A_{I,22})$$

$$\left[B_{22} \psi_2(x_3, k_2) - B_{21} \psi_2(x_3, -k_2) \right]^2 .$$

$$+ \sum_j n_I^B (x_3, k_2^j) - \sum_j n^B (x_3, k_2^j) \tag{D.3}$$

where

$$A_{I,12} A_{22} - A_{12} A_{I,22} = e^{ik_2(2\ell_1 + 2x_2)} \left[(T_{11} R_{21} - R_{11} T_{21}) \right.$$

$$G_{12}^{\ell_1 - x_1} G_{12}^{\ell_1 - x_1} + (T_{11} R_{22} + T_{12} R_{21} - R_{11} T_{22} - R_{12} T_{21}) G_{12}^{\ell_1 - x_1} G_{22}^{\ell_1 - x_1} +$$

$$\left. (T_{12} R_{22} - R_{12} T_{22}) G_{22}^{\ell_1 - x_1} G_{22}^{\ell_1 - x_1} \right] ,$$

$$B_{22}\psi_2(x_3,k_2) - B_{21}\psi_2(x_3,-k_2) = e^{ik_2\ell_3}\left[D_{22}^{\ell_3-x_3} e^{-ik_2x_3}\psi_2(x_3,k_2)\right.$$

$$\left. -D_{21}^{\ell_3-x_3} e^{ik_2x_3}\psi_2(x_3,-k_2)\right],$$

and where

$$M_{I,22}M_{22} = D_{21}^{\ell_3-x_3} D_{21}^{\ell_3-x_3}\left[e^{ik_2}(D_{11}^{x_3}G_{11}^{x_1-1} e^{2ik_2x_2} + D_{12}^{x_3}G_{21}^{x_1-1})\right.$$

$$(T_{11}G_{12}^{\ell_1-x_1} +T_{12}G_{22}^{\ell_1-x_1})+ e^{-ik_2}(D_{11}^{x_3}G_{11}^{x_1-1} e^{2ik_2x_2} +D_{12}^{x_3}G_{22}^{x_1-1})(T_{21}G_{12}^{\ell_1-x_1}$$

$$\left. T_{22}G_{22}^{\ell_1-x_1})\right]\left[e^{ik_2}(D_{11}^{x_3}G_{11}^{x_1-1} e^{2ik_2x_2} +D_{12}^{x_3}G_{21}^{x_1-1}) (R_{11}G_{12}^{\ell_1-x_1}\right.$$

$$+R_{12}G_{22}^{\ell_1-x_1} + e^{-ik_2}(D_{11}^{x_3}G_{11}^{x_1-1} e^{2ik_2x_2} +D_{12}^{x_3}G_{22}^{x_1-1}) (R_{21}G_{12}^{\ell_1-x_1}$$

$$\left. +R_{22}G_{22}^{\ell_1-x_1})\right] e^{ik_2(2\ell_1+2\ell_2)} . \tag{D.4}$$

As ℓ_1 and ℓ_3 go to infinity, the integrand of the integral in Eq. (D.3),
$I(x_1,x_2,x_3,k_2)$ has analytic properties similar to those of the integrand of
the integral in Eq. (B.2). It is an analytic function of k_2, except at the
branch points corresponding to the branch points of $E^{(2)}(k_2)$ and the band edges
of the perfect lattices with the potential $v_1(x)$ and $v_2(x)$ and at the poles
which occur at the zeroes of M_{22} and $M_{I,22}$. We can deform the path of inte-
gration from the real axis to a contour C just below the branch points of
$E^{(2)}(k_2)$. We obtain this asymptotic the contour C for fixed x_1 and x_3:

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$$\left| \int dk_2 I(x_1, x_2, x_3, k_2) \right| < \text{(const.)}_{x_1, x_3} e^{-2h_2^{o} x_2} \text{ as } x_2 \to \infty \qquad (D.5)$$

where h_2^{o} is the distance from the real axis to the branch points of $E^{(2)}(k_2)$.

Again, using Eq. (D.5) and following the same reasoning as we did in Appendix B, we can obtain Eq. (3.14).

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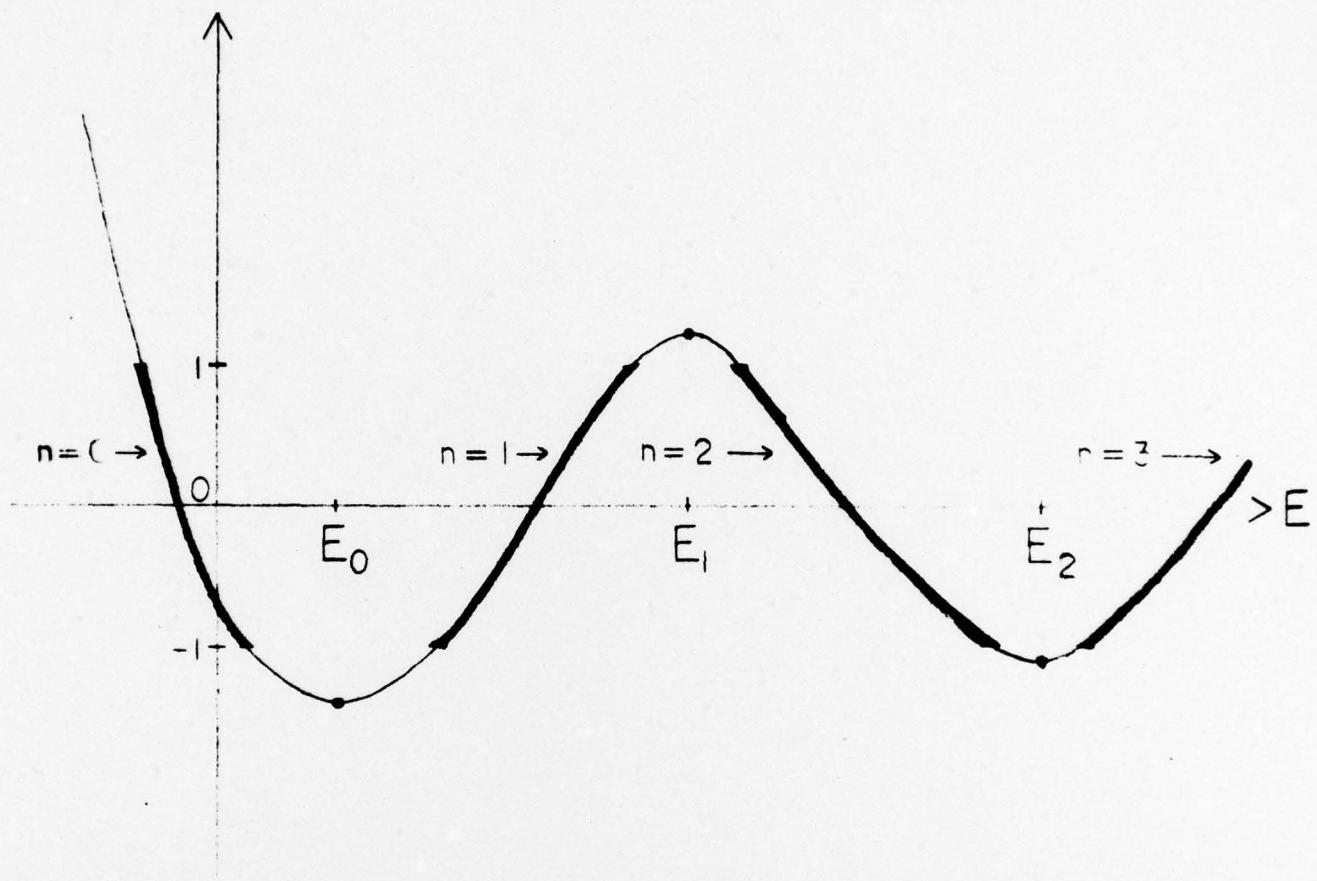
Fig. 1 Schematic version of a Kramer's plot of cos(kb) vs real E . The
energy bands E(n,k) are determined by the regions for which $|\cos(kb)| \leq 1$.
The branch points k^n correspond to the (n+1)th extremum of this plot at
the energy E_n.
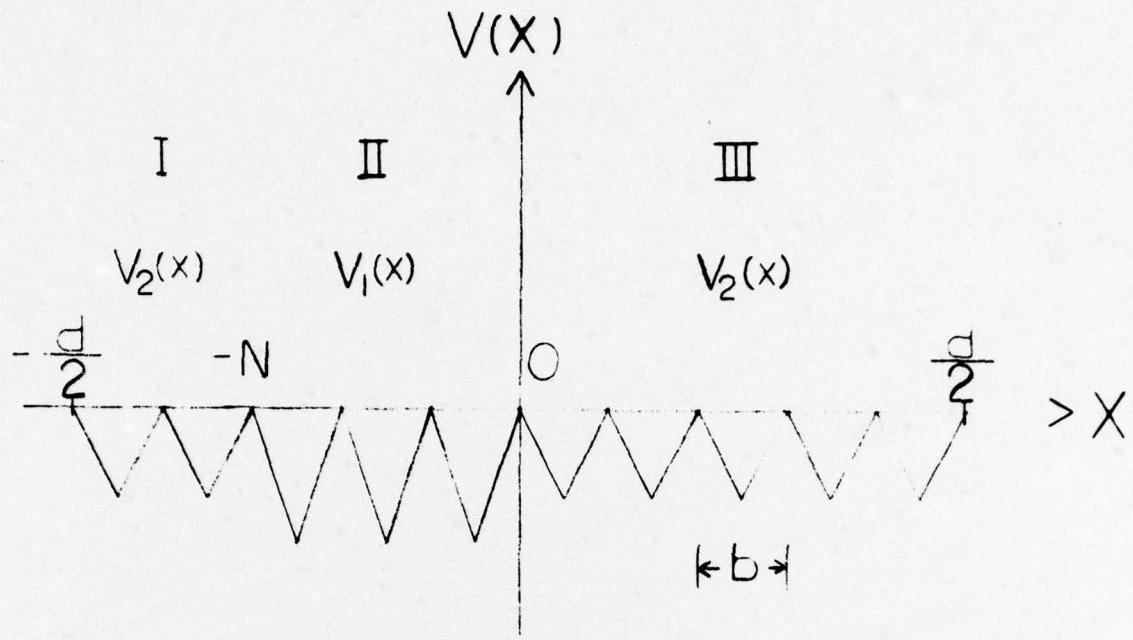
Fig. 2 Schematic plot of the potential $V(x)$ in a fundamental interval $-d/2 \leq x \leq d/2$ ($d \gg N$; $d = 10b$, $N=3b$).
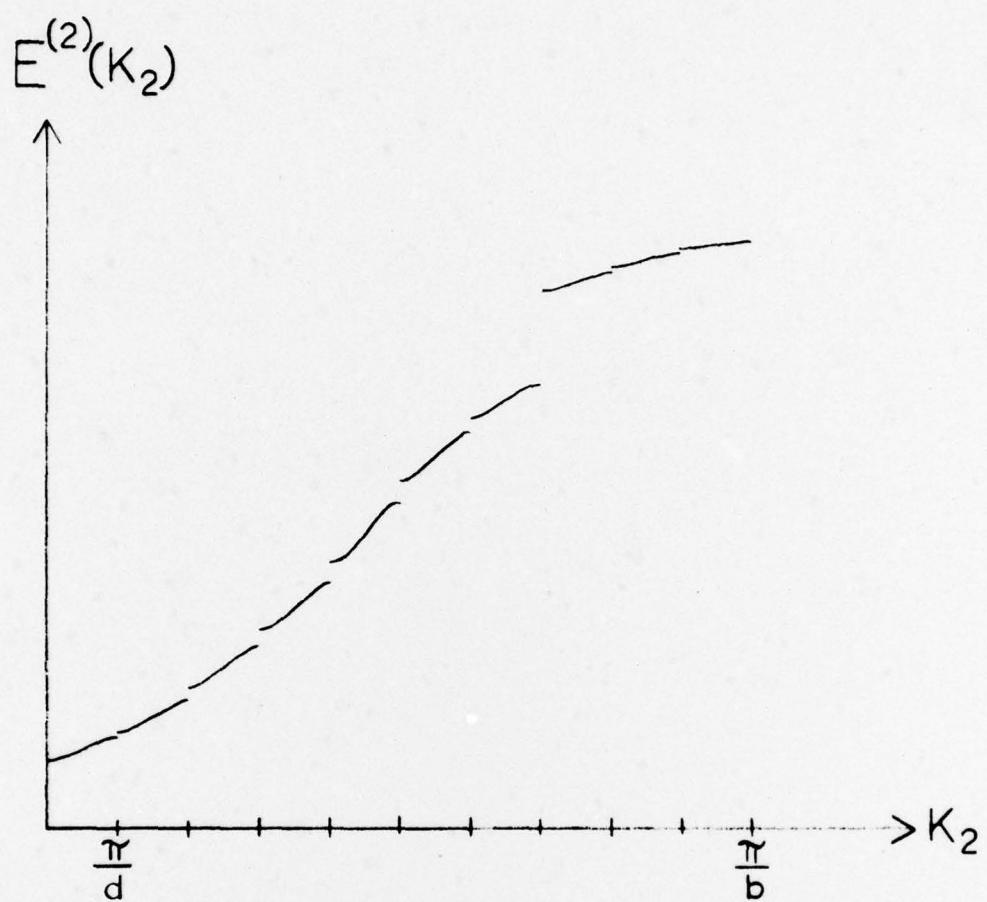
Fig. 3 Schematic plot of the splitting of the original energy band of a perfect lattice with the potential $v_2(x)$ due to the existence of the potential $v_1(x)$ as shown in Fig. 2.
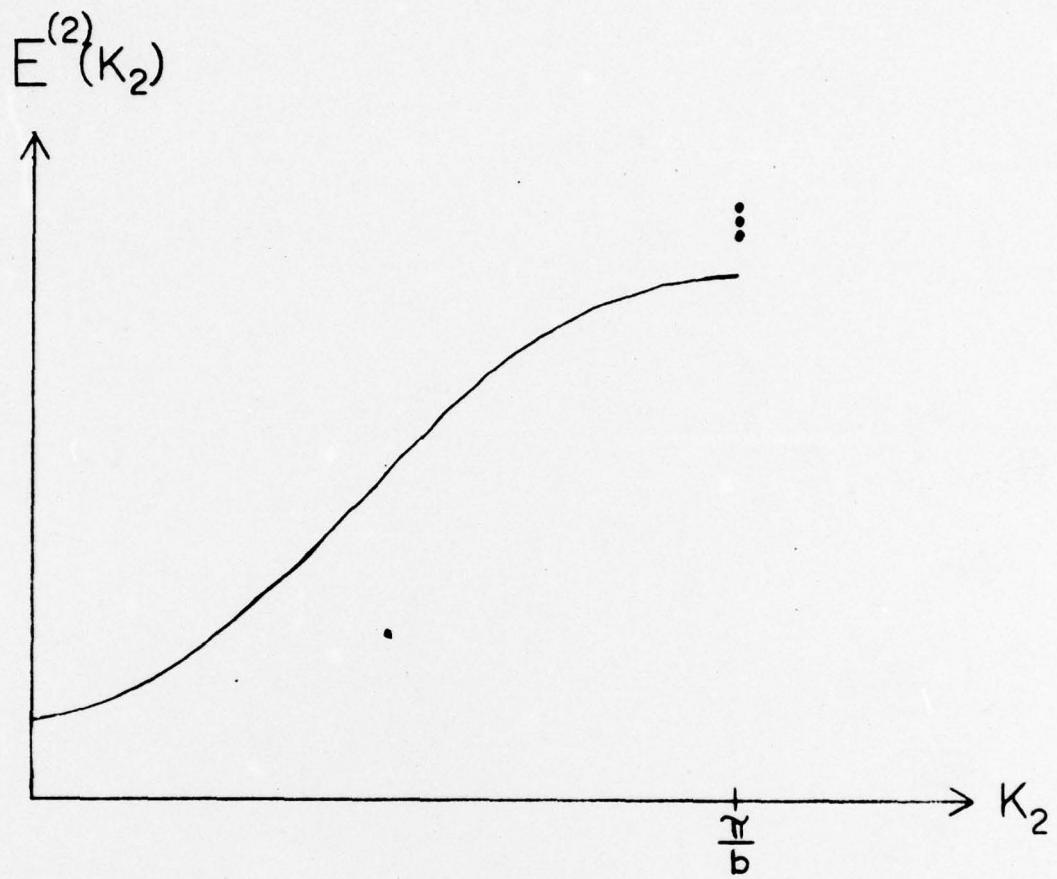
Fig. 4 The same plot as Fig. 3 except d→∞; The dots denote the bound states.
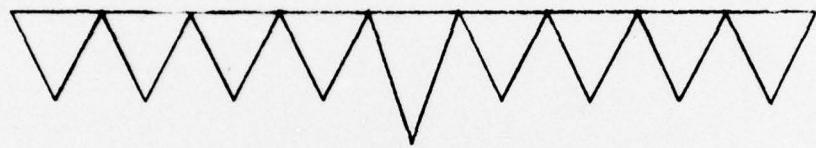
Fig. 5 Schematic plot of an isolated defect in a perfect insulator. The potential strength of the defect is $v_1(x)$.
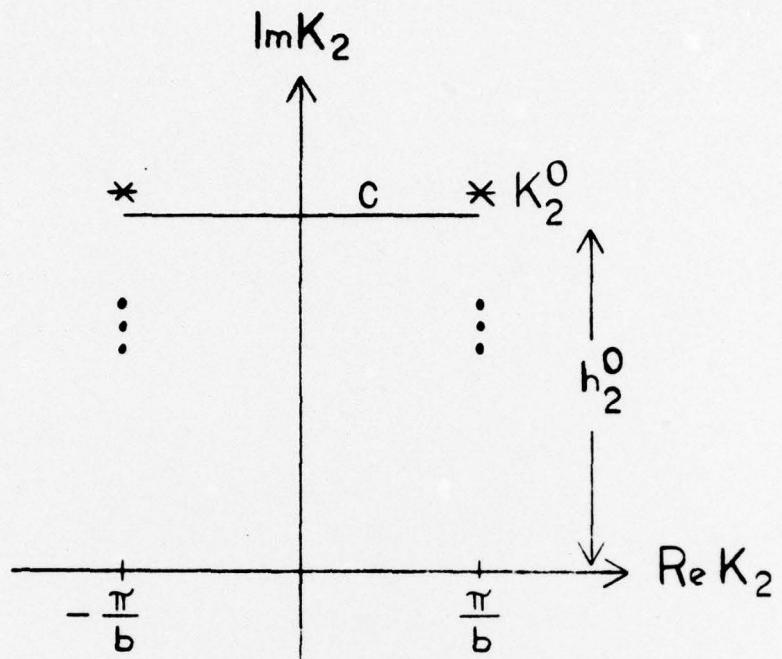
Fig. 6 Integration contour for the integral in Eq. (2.29). The dots indicate the positions of wave vectors k_2^j of the bound states. * indicates the branch points of k_2^0 of the perfect lattice with the potential $v_2(x)$.

insulator 1   interface   insulator 2

$V_1(x)$ $V_2(x)$
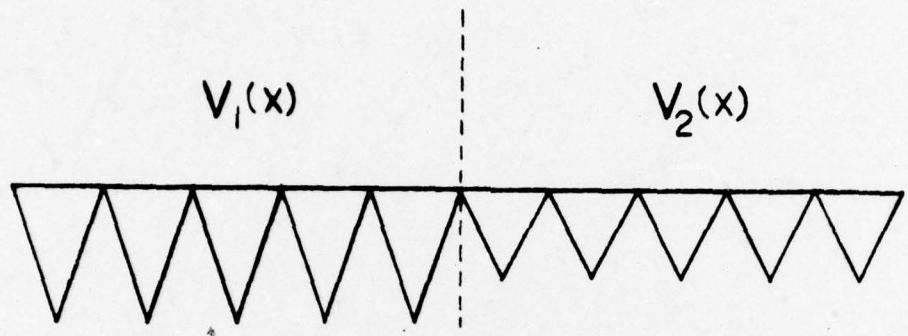
Fig. 7 Schematic plot of an interface between two insulators. The
potentials of insulator 1 and 2 are $v_1(x)$ and $v_2(x)$, respectively.
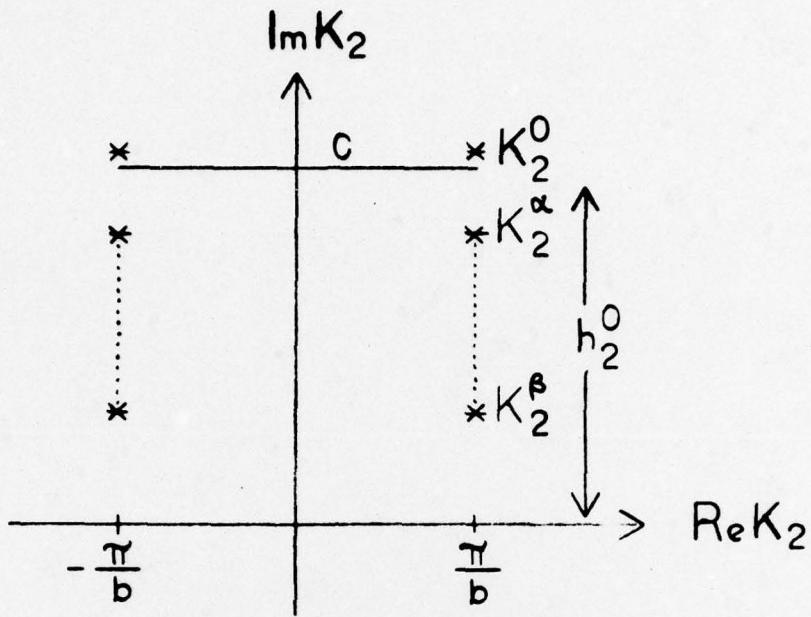
Fig. 8   Integration contour, C, for the integral in Eq. (2.40). k_2^0 is a branch point of $E^{(2)}(k_2)$ in the k_2 plane; k_2^α and k_2^β wavevectors corresponding to the band edges of a perfect lattice with the potential $v_1(x)$. The two closely spaced sequences of points indicate the positions of wavevectors associated with the bound states due to the N cells with potential v_1, embedded in the infinite potential v_2.

interface 1   interface 2

$V_1(x)$ $V_2(x)$ $V_3(x)$

P
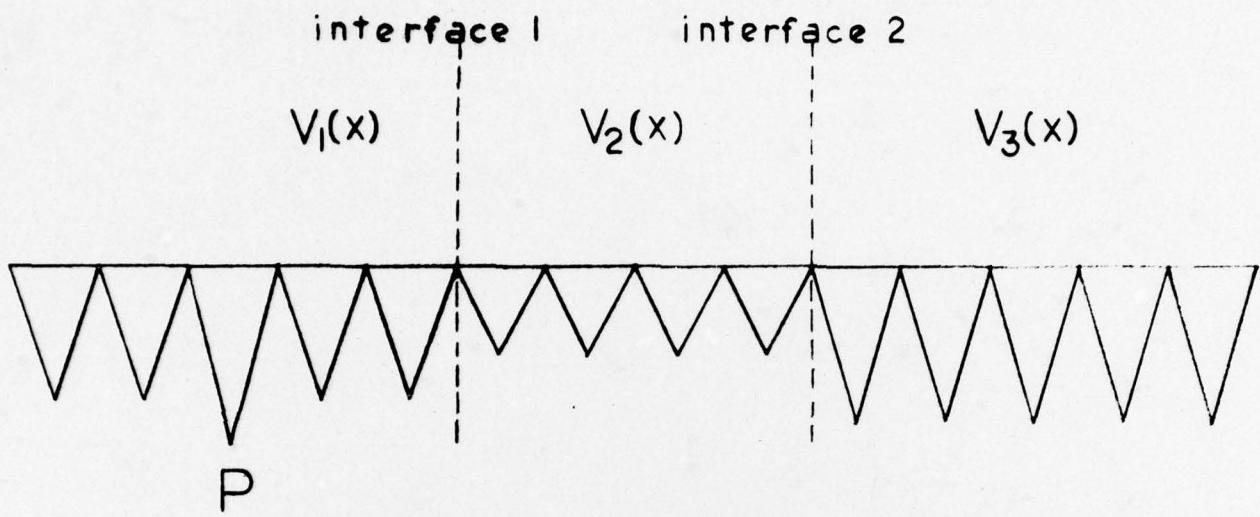
Fig. 9 Schematic plot of n successive insulators with a defect at
the point P .
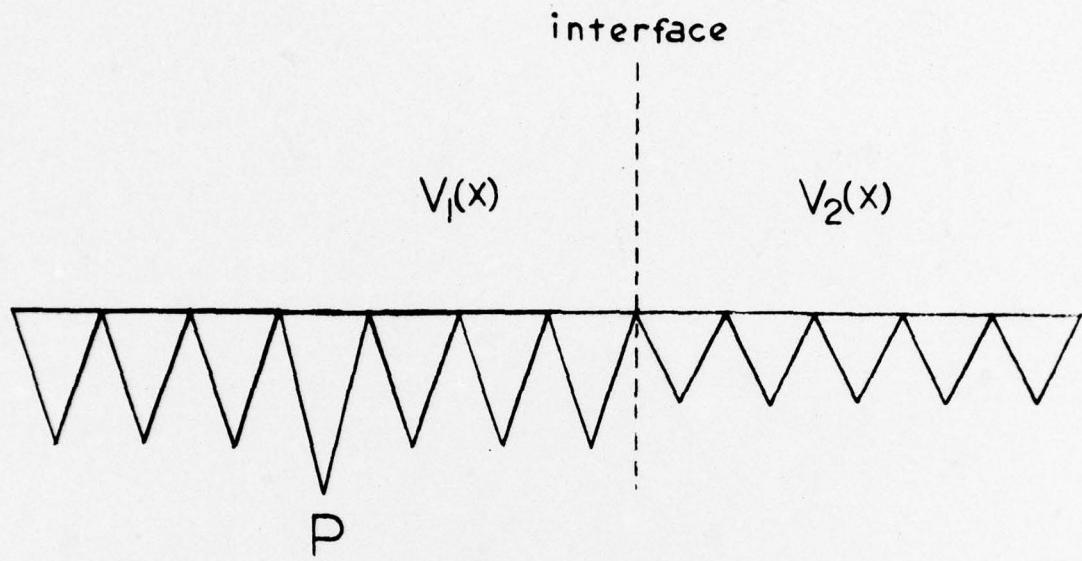
Fig. 10 Schematic plot of an isolated defect at P in a system with an interface.
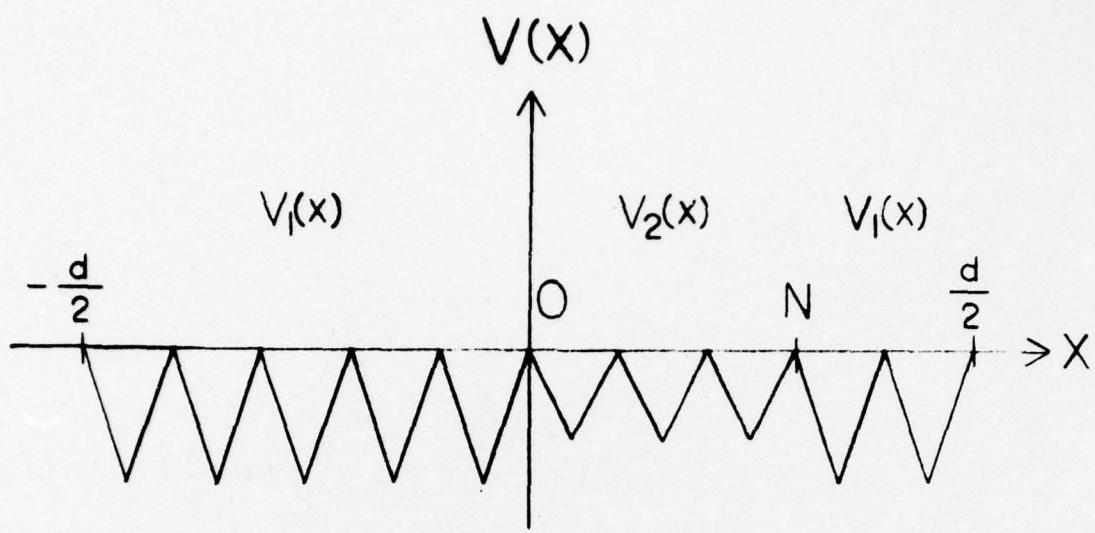
Fig. 11 Schematic plot of the potential V(x) in a fundamental interval
(-d/2 ≤ x ≤ d/2) of the superlattice defined on Eq. (3.8).
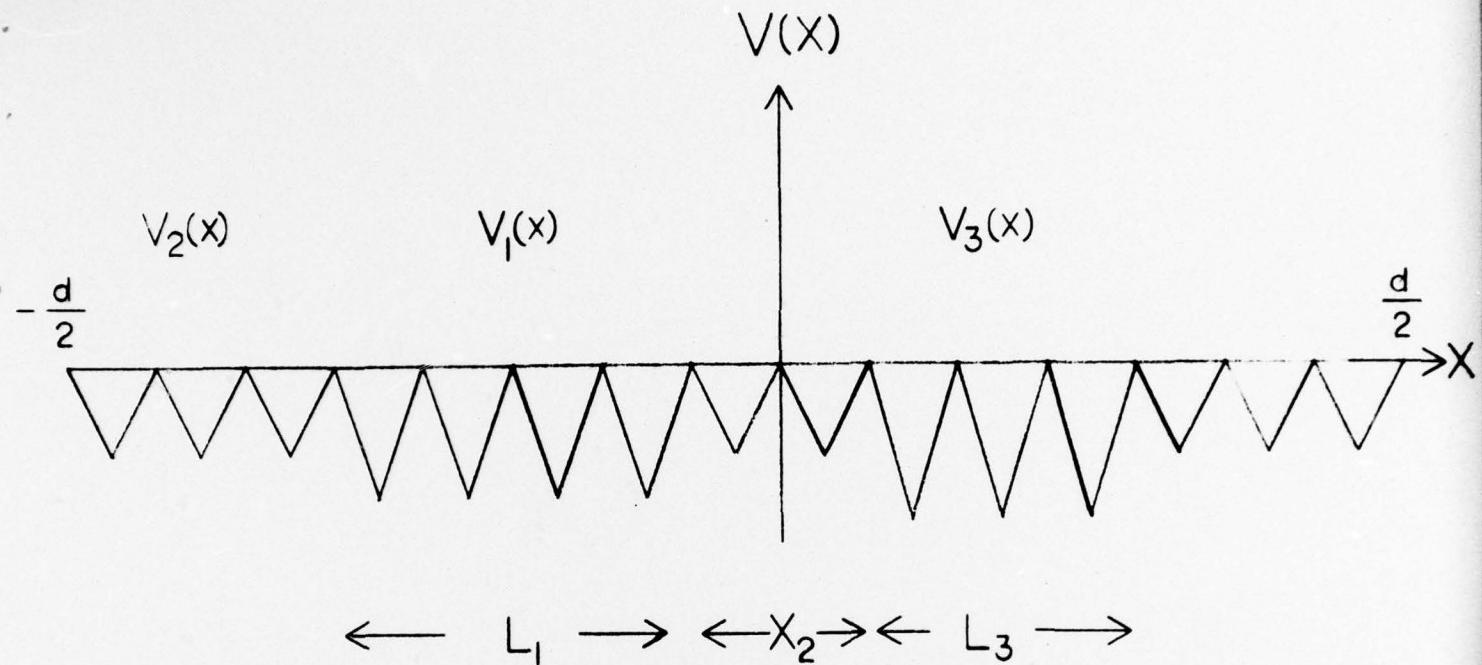
Fig. 12 Schematic plot of the potential $V(x)$ in a fundamental interval of the superlattice which is defined in Appendix D.

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Extending the theory which developed by Kohn, Onffroy and Rehr for a one-dimensional non-periodic system, we have developed a theory that describes how the electronic density distribution near an insulator-insulator interface approaches the bulk behavior. The exponential decay constant depends on the band structure of the two insulators and the positions of localized surface state energies. In addition, we also study the behavior of the electron density perturbation due to a defect across several successive interfaces.